

**FACULTY OF SCIENCES**  
**SYLLABUS**  
**of**  
**Master of Science (Chemistry)**  
**(Semester: I & III)**  
**(Under Continuous Evaluation System)**

**Session: 2020-21**



**The Heritage Institution**  
**KANYA MAHA VIDYALAYA**  
**JALANDHAR**  
**(Autonomous)**

**KANYA MAHA VIDYALAYA JALANDHAR (Autonomous)**

**SCHEME AND CURRICULUM OF EXAMINATION OF TWO-YEAR DEGREE PROGRAMME**

**Master of Science (Chemistry)**

**(Session: 2020-21)**

Master of Science (Chemistry)							
Semester I							
Course Code	Course Name	Course Type	Marks				Examination time (in Hours)
			Total	Ext.		C A	
				L	P		
MCHL-1081	Ligand Field Theory	C	50	40	-	10	3
MCHL-1082	Organic Reaction Mechanism-I	C	50	40	-	10	3
MCHL-1083	Physical Chemistry – Thermodynamics	C	50	40	-	10	3
MCHL-1084	Spectroscopy A: Techniques for Structure Elucidation of Organic Compounds	C	75	60	-	15	3
MCHM-1135	Computer for Chemists – Theory and Practical	C	75	40	20	15	3
MCHP-1086	Inorganic Chemistry Practical (Quantitative Analysis)	C	75	-	60	15	3*2
MCHP-1087	Organic Chemistry Practical	C	75	-	60	15	3*2
Total			450				

**KANYA MAHA VIDYALAYA JALANDHAR (Autonomous)**

**SCHEME AND CURRICULUM OF EXAMINATION OF TWO-YEAR DEGREE PROGRAMME**

**Master of Science (Chemistry)**

**(Session: 2020-21)**

Master of Science (Chemistry)							
Semester-III							
Course Code	Course Name	Course Type	Marks				Examination time (in Hours)
			Total	Ext.		CA	
				L	P		
MCHL-3081	Inorganic Chemistry-II	C	50	40	-	10	3
MCHL-3082	Organic Synthesis	C	50	40	-	10	3
MCHL-3083	Surface and Polymer Chemistry	C	50	40	-	10	3
MCHL-3084	Electrochemistry and Chemical Dynamics	C	50	40	-	10	3
MCHL-3085	Photochemistry and Pericyclic reactions	C	50	40	-	10	3
MCHP-3086	Inorganic Chemistry Practical (Preparations)	C	75	-	60	15	3*2
MCHP-3087	Physical Chemistry Practical	C	75	-	60	15	3*2
Total			400				

## **Programme Specific Outcomes**

On successful completion of this Programme, students will have ability to:

PSO1: do global level research, pursue Ph.D. programme and targeted approach of CSIR-NET examination and competitive exams conducted by service commission

PSO2: attain enormous job opportunities at all levels of chemical, pharmaceutical, food products and life-oriented material industries.

PSO3: get recruitment in R & D and synthetic division of polymer industries & Allied division. PSO4: apply modern methods of analysis to chemical systems in a laboratory setting.

PSO5: work effectively and safely in a laboratory environment, use technologies/instrumentation to gather and analyze data and work in teams as well as independently.

PSO6: think critically, develop scientific temper and analyze various chemical

**Master of Science (Chemistry) (Semester-I)**  
**Session 2020-21**  
**COURSE CODE: MCHL-1081**  
**Course Title: Ligand Field Theory (Theory)**

**Course outcomes:**

Students will be able to

CO1: illustrate an understanding of the principles of theories of metal-ligand bond.

CO2: demonstrate an understanding of spectra of coordination compounds.

CO3: analyze the spectra of transition metal ions.

CO4: analyze Tanabe – Sugano and Orgel diagrams.

CO5: interpret the stability of complexes.

CO6: understand the electronic spectra in transition metal complexes.

CO7: learn mathematical rules for the formation of a group and Point groups

CO8: construct the Character table for various point group and to determine the symmetry of hybrid orbitals

**Master of Science (Chemistry)**  
**(Semester-I)**  
**Session: 2020-21**  
**COURSE CODE: MCHL-1081**  
**COURSE TITLE: Ligand field Theory**

**(Theory)**

**Time: 3 Hrs**

**Max. Marks: 50**

**(Theory: 40, CA: 10)**

**Note: The students are allowed to use Non-Programmable Calculator.**

**Instructions for the Paper Setters:**

Eight questions of equal marks (eight each) are to be set, two in each of the four Sections (A-D). Questions of Sections A-D should be set from UNITs I-IV of the syllabus respectively. Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each section. The fifth question may be attempted from any Section.

**UNIT-I**

**Symmetry**

Symmetry elements, symmetry operations and their matrix representation, group postulates and types, multiplication tables, point group determination, determination of reducible and irreducible representations, character tables, construction of character tables for  $C_{2v}$ ,  $C_{3v}$  (non-abelian group), use of symmetry in obtaining symmetry of orbitals in molecules, use of character table to determine which metal orbitals are used in  $\sigma$  and  $\pi$  bond formation in octahedral, tetrahedral and square planar transition metal complexes, qualitative splitting of s, p, d, f orbitals in octahedral, tetrahedral and square planar fields using character tables and without the use of character tables.

**UNIT-II**

**Molecular Orbital Theory for Metal Complexes:**

Recapitulations, ligands symmetry orbitals and metal orbitals involved in molecular orbitals formation in octahedral complexes, MOEL diagrams for octahedral tetrahedral and square planar complexes showing  $\sigma$  and  $\pi$  bonding in transition metal complexes.

**Interelectronic Repulsions:**

Spin-spin, orbital-orbital and spin orbital coupling, LS and jj coupling schemes, determination of all the spectroscopic terms of  $p^n$ ,  $d^n$  ions, determination of the ground state terms for  $p^n$ ,  $d^n$ ,  $f^n$  ions using L.S. scheme, determination of total degeneracy of terms, order of interelectronic repulsions and crystal field strength in various fields, two type of electron repulsion parameters, spin orbit coupling parameters ( $\lambda$ ) energy separation between different j states, The effect of octahedral and tetrahedral fields on S, P, D and F terms (with help of the character table), splitting patterns of and G, H and I terms

### UNIT-III

#### Free Ions in Medium and Strong Crystal Fields:

Strong field configurations, transition from weak to strong crystal fields, evaluation of strong crystal field terms of  $d^2$  configuration in octahedral and tetrahedral crystal fields (using group theory), construction of the correlation energy level diagrams of  $d^2$  configuration in octahedral field, study of energy level diagrams for higher configurations, selection rules of electronic transitions in transition metal complexes, their proof using group theory, relaxation of the selection rule in centrosymmetric and non-centrosymmetric molecules, Orgel diagrams, Tanabe Sugano diagrams

#### Magnetic Properties:

Van Vleck's formula for susceptibility, first order Zeeman effect, second order Zeeman effect, KT states, quenching of orbital angular momentum by ligand field, the magnetic properties of A and E terms, the magnetic properties of T terms, electronic delocalization, magnetic properties of  $d^n$  and  $f^n$  metal ions.

### UNIT-IV

#### Electronic Spectra of Transition Metal Complexes:

Variation of the Racah parameter, nephelauxetic effect -central field covalency, symmetry restricted covalency, differential radial expansion, spectrochemical series, band intensities, factors influencing band widths, discussion of electronic spectra of octahedral and tetrahedral  $d^1$  –  $d^9$  metal ions, calculation of  $10Dq$  and  $B$  with use of Orgel and Tanabe Sugano diagrams, low spin complexes of  $Mn^{3+}$ ,  $Mn^{2+}$ ,  $Fe^{3+}$ ,  $Co^{3+}$ ,  $Fe^{2+}$ , comment on the spectra of second and third transition series, spectra of  $K_3MoCl_6$  and  $[Rh(NH_3)_6]^{3+}$ , spectra of cis and trans  $[Co(en)_2X_2]^+$ ,  $[Mn(H_2O)_6]^{2+}$ ,  $CuSO_4 \cdot 5H_2O$  and its anhydrous complex, comparison of d–d band with f–f bands. Introduction to Charge Transfer Spectra.

#### Books Recommended:

1. F. A. Cotton, Chemical Application of Group Theory, Wiley Eastern.
2. G. L. Miessler, D. A. Tarr, Inorganic Chemistry, 3<sup>rd</sup> edition, Pearson Education.
3. B. N. Figgis, Introduction to Ligand Field, Wiley Eastern.
4. A. B. P. Lever, Inorganic Electronic Spectroscopy, Elsevier.
5. A. Earnshaw, Introduction to Magnetochemistry, Academic Press.
6. J. E. Huheey, Inorganic Chemistry Principles of Structure and Reactivity, Harper Interscience.
7. R. S. Drago, Physical Method in Chemistry, W.B. Saunders Company.
8. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, Wiley Inter-science.

**Master of Science (Chemistry)**  
**(Semester-I)**  
**Session: 2020-21**  
**COURSE CODE: MCHL-1082**  
**COURSE TITLE: Organic Reaction Mechanism- I (Theory)**

**Course outcomes:**

Students will be able to

CO1: acquire the skills for correct stereochemical assignment and interpretation in simple organic molecules.

CO2: formulate his/her own reasoned opinions in the mechanistic side of organic Reactions

CO3: learn the concept of stereochemistry and its importance

CO3: understand the various types of aliphatic and aromatic nucleophilic substitution reaction and their mechanism

CO4: understand the concept and various types of aromaticity

CO5: know about the stereochemical problems in relation to chemical transformations

CO6: know synthetically the processes relevant organic-chemical reactions and be able to discuss the mechanism of these reactions



**Master of Science (Chemistry)**  
**(Semester-I)**  
**Session: 2020-21**  
**COURSE CODE: MCHL-1082**  
**COURSE TITLE: Organic Reaction Mechanism- I (Theory)**

**Time: 3 hrs**

**Max. Marks: 50**

**(Theory: 40, CA: 10)**

**Note: The students are allowed to use Non-Programmable Calculator.**

**Instructions for the Paper Setters:**

Eight questions of equal marks (eight each) are to be set, two in each of the four Sections (A-D). Questions of Sections A-D should be set from UNITs I-IV of the syllabus respectively. Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each section. The fifth question may be attempted from any Section.

**UNIT-I**

**Nature of Bonding in Organic Reactions:**

Aromaticity in Benzenoid and non-benzenoid compounds. Huckel's Rule, Alternant and non-alternant hydrocarbons. Energy levels of  $\pi$  (pi) molecular orbitals in simple systems. Annulenes, Antiaromaticity, Homoaromaticity, PMO approach.

**Stereochemistry:**

Elements of symmetry, chirality, molecules with more than one chiral center. Threo and erythro isomers, methods of resolution, optical purity. Prochirality – enantiotopic and diastereotopic atoms, groups and faces. Stereospecific and stereoselective synthesis. Asymmetric synthesis. Optical activity in absence of chiral carbon (Biphenyls, Allenes, Spiranes). Chirality due to helical shape.

**UNIT-II**

**Reaction Mechanism, Structure and Reactivity:**

Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, Kinetic and thermodynamic control in product formation. Transition states and reaction intermediates, Isotope effects, Hard and Soft Acid Base concept, Study of reactive intermediates – Types of intermediates, isolation and detection of intermediates (including use of spectral techniques), trapping of intermediates.

**Aliphatic Nucleophilic Substitution – A:**

The  $S_N2$ ,  $S_N1$  and  $S_Ni$  mechanisms, mixed  $S_N1$  &  $S_N2$  mechanism SET mechanism. The neighbouring group mechanism (anchimeric assistance). Neighbouring group participation by pi and sigma bonds.

### UNIT-III

#### **Aliphatic Nucleophilic Substitution – B:**

Classical, non-classical & phenonium cations, Rearrangements in carbocations (general survey). Ester hydrolysis. Nucleophilic substitution at allylic, aliphatic trigonal and vinylic carbon. Effect on the reactivity due to – substrate structure, attacking nucleophile, leaving group and reaction medium. Ambident nucleophiles and substrates, regioselectivity. Meyer's synthesis of aldehydes, ketones, acids and esters. Alkylation by organoboranes.

#### **Aliphatic Electrophilic Substitution:**

Bimolecular mechanism – SE2 and SE1. The SE1 mechanism, Hydrogen exchange, electrophilic substitution accompanied by double bond shifts, diazo-transfer reaction, formation of sulphur ylides, effect of substrates, leaving group and solvent polarity on the reactivity.

### UNIT-IV

#### **Aromatic Electrophilic Substitution:**

The arenium ion mechanism, orientation and reactivity in mono substituted and di substituted aromatics. Energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles. Diazo coupling, Vilsmeier reaction, Gattermann-Koch reaction, Pechmann reaction, Houben – Hoesch reaction, Fries rearrangement.

#### **Aromatic Nucleophilic Substitution:**

SNAr, SN1, benzyne and SRN1 mechanisms. Reactivity effect of substrate structure, leaving group and nucleophile. The von Richter, Sommelet-Hauser, and Smiles rearrangements.

#### **Books Recommended:**

1. Stereochemistry - Eliel
2. Advanced Organic Chemistry – Jerry March.
3. Advanced Organic Chemistry, F. A. Carey, R. J. Sundberg, Volume I and II
4. Highlights of Organic Chemistry, W.J. L. Nobel; An Advanced Text Book.
5. Stereochemistry conformation and Mechanism – P. S. Kalsi

**Master of Science (Chemistry)**  
**(Semester-I)**  
**Session: 2020-21**  
**COURSE CODE: MCHL-1083**  
**COURSE TITLE: Physical Chemistry – Thermodynamics (Theory)**

**Course outcomes:**

Students will be able to

CO1: calculate change in thermodynamic properties, equilibrium constants, partial molar quantities, chemical potential. Identify factors affecting equilibrium constant.

CO2: apply phase rule and, draw phase diagrams for one, and two component systems, identify the dependency of temperature and pressure on phase transitions, and identify first/second order phase transitions.

CO3: solve problems based on Debye-Huckel limiting law, calculate excess thermodynamic properties.

CO4: calculate the absolute value of thermodynamic quantities (U, H, S, A, G) and equilibrium constant (K) from spectroscopic data.

CO5: predict heat capacity ( $C_v$ ,  $C_p$ ) of an ideal gas of linear and non-linear molecules from the number of degrees of freedom, rotational and vibrational wave numbers.

CO6: derive the temperature dependence of the second Virial coefficient (real gases) from interatomic potentials.

CO7: explain  $T^3$  dependence of heat capacity of solids at low temperatures (universal feature) using Debye and Einstein theory of heat capacity of solids.

CO8: explain the concept of Fermi energy in metals and use it to calculate the chemical potential of conduction.

**Master of Science (Chemistry)**  
**(Semester-I)**  
**Session: 2020-21**  
**COURSE CODE: MCHL-1083**  
**COURSE TITLE: Physical Chemistry –Thermodynamics (Theory)**

**Time: 3 Hrs.**

**Max. Marks: 50**

**(Theory: 40, CA: 10)**

**Note: The students are allowed to use Non-Programmable Calculator. Instructions for the Paper Setters:**

Eight questions of equal marks (eight each) are to be set, two in each of the four Sections (A-D). Questions of Sections A-D should be set from UNITs I-IV of the syllabus respectively. Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each section. The fifth question may be attempted from any Section.

**UNIT-I**

**Classical Thermodynamics**

Brief resume of concepts of thermodynamics, free energy, chemical potential and entropy. Partial molar properties, partial molar free energy, partial molar volume and partial molar heat content and their significances. Determination of these quantities. Concept of fugacity and determination of fugacity.

**UNIT-II**

**Non-ideal systems**

Excess functions for non-ideal solutions. Activity, activity coefficients, Debye-Huckel theory for activity coefficient of electrolytic solutions, determination of activity and activity coefficients, ionic strength. Application of phase rule to three component system, second order phase transitions.

**Statistical Thermodynamics:**

Concept of distribution law, thermodynamic probability and most probable distribution, Ensemble averaging, postulates of ensemble averaging. Canonical, grand canonical and micro canonical ensembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers).

**UNIT-III**

**Partition functions**

Translational, rotational, vibrational and electronic partition function, calculation of thermodynamic properties in terms of partition functions. Application of partition functions.

Heat capacity behavior of solids-chemical equilibria and equilibrium constants in terms of partition functions, Fermi-Dirac statistics, distribution laws, and application to metals. Bose-Einstein statistics- distribution law and application to helium.

#### **UNIT-IV**

##### **Non Equilibrium Thermodynamics:**

Thermodynamic criteria for non-equilibrium states, entropy production and entropy flow, entropy balance equations for different irreversible processes (e.g., heat flow, chemical reaction etc.) transformations of generalized fluxes and forces, non-equilibrium stationary states, phenomenological equations, microscopic reversibility and Onsager's reciprocity relations, electro kinetic phenomena, diffusion, electric conduction, irreversible thermodynamics for biological systems, coupled reactions.

##### **Books Recommended:**

1. I F Nash: Elements of classical and statistical thermodynamics
2. Lee Bot: Irreversible thermodynamics
3. Thermodynamics of Biological Processes, D. Jou and J.E. Lee Bot
4. I Prigogine: Introduction to thermodynamics of irreversible processes
5. T L Hill: Introduction to statistical thermodynamics.

**Master of Science (Chemistry)**  
**(Semester-I)**  
**Session: 2020-21**  
**COURSE CODE: MCHL-1084**  
**COURSE TITLE: SPECTROSCOPY – A: Techniques in Structure Elucidation of Organic**  
**Compounds**  
**(Theory)**

**Course outcomes:**

Students will be able to

CO1: learn about the Principle and applications of ultraviolet and Woodward Fisher Rule

CO2: understand the infra-red spectroscopy in organic structure determination

CO3: know about the Nuclear magnetic resonance spectroscopy. Proton chemical shift, spin-spin coupling, coupling constants and applications to organic structures  $^{13}\text{C}$  resonance spectroscopy

CO4: learn the Mass spectrometry and its applications

CO5: to know about the Vibrational spectroscopy, Vibrational coupling overtones and Fermi resonance.

CO6: apply NMR, IR, MS, UV-Vis spectroscopic techniques in solving structure of organic molecules and in determination of their stereochemistry.

CO7: interpret the above spectroscopic data of unknown compounds.

CO8: use these spectroscopic techniques in their research.

**Master of Science (Chemistry)**  
**(Semester-I)**  
**Session: 2020-21**  
**COURSE CODE: MCHL-1084**  
**COURSE TITLE: SPECTROSCOPY – A: Techniques in Structure Elucidation of Organic Compounds (Theory)**

**Max. Marks: 75**

**Time: 3 hrs.**

**(Theory: 60, CA: 15)**

**Note: The students are allowed to use Non-Programmable Calculator.**

**Instructions for the Paper Setters:**

Eight questions of equal marks (twelve each) are to be set, two in each of the four Sections (A-D). Questions of Sections A-D should be set from UNITs I-IV of the syllabus respectively. Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each section. The fifth question may be attempted from any Section.

**UNIT-I**

**Nuclear Magnetic Resonance**

The Nuclear spin, Larmor frequency, the NMR isotopes, population of nuclear spin level, spin and spin lattice relaxation. Measurement techniques (CW & FT method), solvent used. Chemical shift, reference compounds, shielding constant, range of typical chemical Shifts simple application of chemical shifts, ring current and aromaticity. Shifts for  $^1\text{H}$  and  $^{13}\text{C}$ . - Spin-spin interactions, Low and High resolution spectra with various examples, Correlation of H bound to carbon, H bound to other nuclei such as nitrogen, oxygen, sulphur, Complex spin-spin interaction, between two or more nuclei. Effect of chemical exchange, fluxional molecules, Hindered rotation on NMR spectrum Karplus relationship, nuclear magnetic double resonance, chemically induced dynamic nuclear polarization. Brief introduction to multipulse NMR spectroscopy, Application of structure elucidation of simple organic molecules Lanthanide shift.

**UNIT-II**

**Mass Spectroscopy**

Elementary theory - Measurement techniques (EI, CI, FD, FAB), Resolution, exact masses of nuclides, Molecular ions, isotope ions, fragment ions of odd and even electron types, rearrangement ions, Factors affecting cleavage patterns, simple cleavage, cleavages at a hetero atom, multicentre fragmentations rearrangements, Reteroiels – Alder fragmentation. Cleavage associated with common functional groups (Aldehydes, ketones cyclic and acyclic esters, alcohols, olefins, aromatic compounds amines). - Special methods of GCMS, high resolution MS, Introduction to radical anion mass spectroscopy. Interpretation of the spectrum of an unknown.

**Ultraviolet and Visible Spectroscopy**

The energy of electronic excitation, measurement techniques, Beer-Lambert Law, Molar extinction coefficient. The Frank Condon Principle. Different types of transition noticed in UV spectrum of organic functional groups and their relative energies. Chromophore, auxochromes, factors affecting max, Effect of steric hindrance to coplanarity, Solvent Effects. Applications of U.V. spectroscopy.

### **UNIT-III**

#### **Infrared Spectroscopy**

Vibrational Energy Levels, Selection Rules, Force Constant, Fundamental Vibration Frequencies, Factors influencing Vibrational Frequencies (Vibrational Coupling, Hydrogen Bonding, Electronic effect, Bond Angles, Field Effect). Sampling Techniques, Absorption of Common functional Groups, Interpretation, Finger print Regions.

#### **Applications in Organic Chemistry**

- (a) Determining purity and quantitative analysis.
- (b) Studying reaction kinetics.
- (c) Determining purity and quantitative analysis.
- (d) Studying hydrogen bonding.
- (e) Studying molecular geometry & conformational analysis.
- (f) Studying reactive species

### **UNIT-IV**

#### **1. Solution of Structural Problems by Combined Use of the following Spectroscopic Techniques:**

- (a) Electronic spectra
- (b) Vibrational spectroscopy
- (c) NMR ( $^1\text{H}$  and  $^{13}\text{C}$ ) spectroscopy
- (d) Mass Spectroscopy

#### **Books Recommended:**

1. W. Kemp. Organic Spectroscopy.
2. W. Kemp. N.M.R. Spectroscopy.
3. D.H. Williams and I. Fleming. Spectroscopic Methods in Organic Chemistry.
4. R.M. Silverstein & G.C. Bassler, Spectrometric Identification of Organic Compounds.
5. Introduction to Spectroscopy – Pavia



**Master of Science (Chemistry)**  
**(Semester-I)**  
**Session: 2020-21**  
**COURSE CODE: MCHM-1135**  
**COURSE TITLE: Computer for Chemists**

**Course outcomes:**

At the end of the course, the learners should be able to:

CO1: write short simple programs in C language and be able to compile and execute them in a host of machines.

CO2: use standard software tools to perform algebraic and numerical calculations often required in elementary physical chemistry in the areas of quantum chemistry, spectroscopy, kinetics and thermodynamics

**Master of Science (Chemistry) Semester - I**  
**Session 2020-21**

**(Theory)**  
**COMPUTER FOR CHEMISTS**  
**Course code: MCHM - 1135**

**Examination Time: (3+3) Hours**

**Max. Marks: 75**  
**Theory: 40**  
**Practical: 20**  
**CA: 15**

**Note: The students are allowed to use Non-Programmable Calculator.**

**Instructions for Paper Setter -**

Eight questions of equal marks (8 marks each) are to set, two in each of the four sections (A-D). Questions of Sections A-D should be set from Units I-IV of the syllabus respectively. Questions may be divided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each section. The fifth question may be attempted from any section.

**1. Computer Programming in C language (30 Hrs.)**

**UNIT-I**

Principles of programming, algorithms and flowcharts.

Elementary programming, a typical C program, print function.

Introduction of declarations, assignments and variables: concept of an integer, concept of a variable, rules for naming variables, assignment statement, arithmetic operators.

Integer arithmetic expressions, truncation effects, relative priority of arithmetic operators, use of parenthesis, modulus operator.

**UNIT-II**

Floating point numbers, scientific notation, converting integers to floating point and vice versa, coercion and cast operator, type char.

Decision making in C, scanf function, relational operators, logical operators, if statement, if else statement, nesting of if statement.

### **UNIT-III**

The while loop, do while loop, for loop, nesting of for loop.

Type char and ASCII code, character strings and how to print them, octal and hexadecimal notation.

User defined functions, returning value from a function, functions with more than one parameters.

### **UNIT-IV**

Arrays, declaring an array, initializing an array, break statement, strings and character arrays, sorting an array, finding maximum and minimum in an array, multidimensional arrays. Input and output.

## **2.Computer programs in Chemistry (15Hrs. )**

### **(these are to be done in the practical class)**

Development of small computer codes involving simple formulae in chemistry:

#### **UNIT - I**

1. Calculation of mean, median, mode.
2. Solution of a quadratic equation.
3. Calculation of linear regression.
4. Calculation of curve linear regression.

#### **UNIT - II**

5. Calculation of Bohr orbit from de Broglie Lambda for electron.
6. Calculation of wave number and frequency from value of wavelength.
7. Calculation of van der Waals radii.
8. Radioactive decay.
9. Rate constant of a 1st order reaction, 2nd order reaction.
10. Determination
11. Calculation of lattice energy using Born Land e equation.

#### **UNIT - III**

12. Addition, multiplication and solution of inverse of 3 X 3 matrix.
13. Calculation of average molecular weight of a polymer containing  $n_1$  molecules of molecular weight  $m_1$ ,  $n_2$  molecules of molecular weight  $M_2$  and soon.
14. Program for calculation of molecular weight of organic compound containing C, H, N, O and S.

15. Calculation of reduced mass of diatomic molecule.
16. Calculate the RMS and most probable velocity of a gas.

#### **UNIT - IV**

17. Calculate the ionic mobility from ionic conductance values.
18. Determine the thermodynamic parameters for isothermal expansion of monoatomic ideal gas.
19. Calculation of value of g- factor from value of J and S.
20. Calculate the bond length and bond angles using crystal structure data.

#### **References / Textbooks:**

1. K.V. Raman, Computers in Chemistry, Tata McGraw Hill, 1993.
2. Henry Mullish, Herbert L. Cooper, The Spirit of C: An Introduction to Modern Programming, Jaico Publications, 1987.
3. Anshuman Sharma, Learn Programming in C, Lakhanpal Publishers, 7th Edition.
4. E Balagurusamy, Programming in ANSI C, Tata McGraw-Hill, 2002.
5. Yashvant Kanetkar, Let Us C, BPB Publications, 2016.
6. Byron Gottfried, Schaum's Outline Programming with C, McGraw Hill, 1996.

Note: The latest editions of the books should be followed.

**Master of Science (Chemistry)**  
**(Semester-I)**  
**Session: 2020-21**  
**COURSE CODE: MCHP-1086**  
**COURSE TITLE: INORGANIC CHEMISTRY (PRACTICAL)**  
**(Quantitative Analysis)**

**Time: 60 hrs.**

**Max. Marks: 75**  
**(P: 60, CA: 15)**

**Instruction for practical examiner:** Question paper is to be set on the spot jointly by the Internal and External Examiners. Two copies of the same should be submitted for the record to COE Office, Kanya Maha Vidyalaya, Jalandhar.

**I. Oxidation-Reduction Titrations**

1. Standardization with sodium oxalate of  $\text{KMnO}_4$  and determination of  $\text{Ca}^{2+}$  ion.
2. Standardization of ceric sulphate with Mohr's salt and determination of  $\text{NO}_3^{-1}$  and  $\text{C}_2\text{O}_4^{2-}$  ions.
3. Standardization of  $\text{K}_2\text{Cr}_2\text{O}_7$  with  $\text{Fe}^{2+}$  and determination of  $\text{Fe}^{3+}$  (Ferric alum)
4. Standardization of hypo solution with potassium iodate /  $\text{K}_2\text{Cr}_2\text{O}_7$  and determination of available  $\text{Cl}_2$  in bleaching powder,  $\text{Sb}^{3+}$  and  $\text{Cu}^{2+}$ .
5. Determination of hydrazine with  $\text{KIO}_3$  titration.

**II. Precipitation Titrations**

1.  $\text{AgNO}_3$  standardization by Mohr's method by using adsorption indicator.
2. Volhard's method for  $\text{Cl}^-$  determination.
3. Determination of ammonium / potassium thiocyanate.

**III. Complexometric Titrations**

1. Determination of  $\text{Mg}^{2+}$  and  $\text{Mn}^{2+}$  in a mixture using fluoride ion as a demasking agent.
2. Determination of  $\text{Ni}^{2+}$  (back titration).
3. Determination of  $\text{Ca}^{2+}$  (by substitution method).

**IV. Gravimetric Analysis**

1. Determination of  $\text{Ba}^{2+}$  as its chromate.
2. Estimation of lead as its lead molybdate.
3. Estimation of chromium (III) as its lead chromate.
4. Estimation of  $\text{Cu}^{2+}$  using Ammonium/ Sodium thiocyanate.

**Books Recommended:**

Vogel's book on Inorganic Quantitative Analysis.

**Master of Science (Chemistry)**  
**(Semester I)**  
**Session: 2020-21**  
**COURSE CODE: MCHP-1087**  
**COURSE TITLE: ORGANIC CHEMISTRY**  
**(PRACTICAL)**

**Course outcomes:**

The students will be able to

CO1: independently perform two step organic synthesis.

CO2: identify the synthesized compounds by TLC

CO3: perform analysis of common analgesic drugs by TLC

CO4: extract, identify and characterize the compounds isolated from natural products

**Master of Science (Chemistry)**  
**(Semester I)**  
**Session: 2020-21**  
**COURSE CODE: MCHP-1087**  
**COURSE TITLE: ORGANIC CHEMISTRY (PRACTICAL)**

**Time: 6 Hrs.**

**Max. Marks: 75**  
**(P: 60, CA: 15)**

**Instruction for practical examiner:** Question paper is to be set on the spot jointly by the Internal and External Examiners. Two copies of the same should be submitted for the record to COE Office, Kanya Maha Vidyalaya, Jalandhar.

**UNIT-I**

1. **Purification and Characterization of Organic Compounds**, the student is expected to carry out the experiments of purification (fractional crystallization, fractional distillation, chromatography) separation, purification and identification of the compounds of binary organic mixture (liquid-liquid, liquid-solid and solid-solid), using chemical analysis and IR and PMR spectral data. The student should also check the purity of the separated components on TLC plates.
2. To carry out the analysis of common analgesic drugs by thin layer chromatography, Acetaminophen, Aspirin, caffeine, phenacetin, salicylamide. (Learn to check purity of the given samples and completion of the chemical reactions).

**UNIT-2**

**Organic Synthesis and Extraction of Organic Compounds from Natural Sources.** The student is expected to carry out 4 to 6 organic preparations (usually involving not more than two steps), some of the illustrative experiments are listed below:-

1. *Extraction of Caffeine from tea leaves*  
(Ref. Experiment Organic Chemistry, (H. Dupont Durst, George W. Gokel, P 464 McGraw Hill Book Co., New York).  
Student would be asked to purify crude sample, check the purity on a TLC single spot and get the NMR scanned and interpret (Three methyl singlets and 1 methane singlet).
2. *Isolation of casein from milk* (try some typical colour reactions proteins).
3. *Synthesis of 2-phenylindole-Fischer Indole Synthesis*. Book 1, p. 852  
**Aim:** To Study condensation and cyclization reactions.
4. *Synthesis of 3-nitrobenzoic from benzoic acid* (Rf. Ibid., p.245-247 and 443-448). **Aim:** To demonstrate the process of meta nitration, esterification and saponification of an ester. Make a comparative study of IR and PMR spectra of benzoic acid, methyl benzoate, methyl 3-nitrobenzoate.
5. *Cannizzaro's reaction of 4-chlorobenzaldehyde*. Book 1, p 760  
**Aim:** To demonstrate technique of isolation of two products from the reaction mixture and the procedure of intermolecular hydride transfer. Make a comparative study of IR and PMR spectra of 4 chlorobenzaldehyde, 4-chlorobenzoic acid 4-chlorobenzyl alcohol.
6. *Synthesis of 1,3,5-Tribromobenzene from aniline*. **Aim:** To demonstrate: Bromination, Diazotization and Reduction.

**Books Recommended:**

Vogel's Textbook of practical organic chemistry, 5<sup>th</sup> edition

**Master of Science (Chemistry)**  
**(Semester-III)**  
**Session: 2020-21**  
**COURSE CODE: MCHL-3081**  
**COURSE TITLE: Inorganic Chemistry-II**  
**(Theory)**

**Course outcomes:**

Students will be able to

CO1: know about the various metal ions present in our body, their function in body and role in medicine

CO2: learn about the different enzymes participating in the chemical reactions inside the body and their functions

CO3: study about the different oxygen carriers present in the body with their structure and stereochemistry

CO4: study in detail about nitrogen fixation reactions and microorganisms involved in nitrogen fixation reactions



**Master of Science (Chemistry)**  
**(Semester-III)**  
**Session: 2020-21**  
**COURSE CODE: MCHL-3081**  
**COURSE TITLE: Inorganic Chemistry-II**  
**(Theory)**

**Time: 3 Hrs**

**Max. Marks: 50**

**(Theory: 40, CA: 10)**

**Note: The students are allowed to use Non-Programmable Calculator.**

**Instructions for the Paper Setters:**

Eight questions of equal marks (eight each) are to be set, two in each of the four Sections (A-D). Questions of Sections A-D should be set from UNITs I-IV of the syllabus respectively. Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each section. The fifth question may be attempted from any Section.

**UNIT-I**

**Metal Ions in Biological Systems-** Essential and trace elements, periodic survey of essential and trace elements, biological importance and relative abundance,  $\text{Na}^+$  /  $\text{K}^+$  ion pump.

**Transport and Storage of Dioxygen-** Oxygen carriers-Hb and Mb: Structure and mechanism of their function, co-operativity, inhibition and poisoning by ligands and metal ions, hemocyanins and hemerythrin, model complexes of iron, cobalt and copper.

**UNIT-II**

**Bioenergetics and ATP Cycle-** Process concept to phosphate hydrolysis, Nucleotide transfer- DNA polymerase, phosphate transfer pyruvate kinase, phosphoglucomutase, creatine kinase, ATPase  
**Photosynthesis and respiration** – chlorophyll: structure, function and its synthetic model.

**Bio redox Agents and Mechanism-** Enzymes and their functioning, Vitamin B<sub>12</sub> coenzyme, its function and application in organic syntheses, intake of alcohol and its remedy.

**UNIT-III**

**Biochemistry of Iron-** Availability of iron, competition for iron, iron toxicity and nutrition.

**Electron Transfer in Biology-** Cytochromes-structure and function,  $\text{CN}^-$  and CO poisoning, Ferredoxin and rubredoxin. **Nitrogenase-** Biological  $\text{N}_2$  fixation, molybdenum nitrogenase, spectroscopic and other evidence, other nitrogenases model systems.

**Metal Storage, Transport-** Ferritin, transferring and siderophores.

**UNIT-IV**

**Metalloenzymes-** Zinc enzymes-carboxypeptidase and carbonic anhydrase, Copper enzymes- superoxide dismutase.

**Calcium in Biology-** Calcium in living cell, transport and regulation, molecular aspects of intramolecular processes,

**Metals in Medicine-** Metal deficiency and disease, toxic effects of antibiotics and related compounds, chelate therapy

**Books Recommended:**

1. Principles of Bioinorganic Chemistry, S. J. Lippard and Berg, University Science Books.
2. Inorganic Biochemistry, Vol I and II. Ed. G. L. Eichhorn, Elsevier.
3. J.E. Huheey : Inorganic Chemistry III & IV Ed. Pearson Education Asia – (2002).
4. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, 5<sup>th</sup> Edition.
5. Progress in Inorganic Chemistry, Vols 18 and 38 Ed. J. J. Lippard, Wiley
6. Bioinorganic Chemistry by D.Banerjia

**Master of Science (Chemistry)**  
**(Semester-III)**  
**Session: 2020-21**  
**COURSE CODE: MCHL-3082**  
**COURSE TITLE: Organic Synthesis**  
**(Theory)**

**Course outcomes:**

Students will be able to

CO1: understand general mechanistic consideration of organic rearrangements

CO2: understand synthesis and reactions of macro ring compounds and fused polynuclear hydrocarbons

CO3: study the synthesis and reactions of three, four, six, seven and large membered Heterocycles

CO4: know about the use of various reagents in organic synthesis and functional group transformations

CO5: understand the basic concepts of supramolecular chemistry

**Master of Science (Chemistry)**  
**(Semester-III)**  
**Session: 2020-21**  
**COURSE CODE: MCHL-3082**  
**COURSE TITLE: Organic Synthesis (Theory)**

**Time: 3 Hrs**

**Max. Marks: 50**

**(Theory: 40, CA: 10)**

**Note: The students are allowed to use Non-Programmable Calculator.**

**Instructions for the Paper Setters:**

Eight questions of equal marks (eight each) are to be set, two in each of the four Sections (A-D). Questions of Sections A-D should be set from UNITS I-IV of the syllabus respectively. Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each section. The fifth question may be attempted from any Section.

**UNIT-I**

**Rearrangements:** General mechanistic considerations – nature of migration, migratory aptitude, memory effects. A detailed study of the following rearrangements: Pinacol-pinacolone, Wagner-Merwein, Demjanov, Benzil-Benzilic acid, Favorskii, Arndt-Eistert synthesis, Neber, Beckmann, Hofmann, Curtius, Schmidt, Baeyer-Villiger, Shapiro reaction.

**Polynuclear Compounds & Macro-Ring Compounds**

Introduction, comparative study of aromatic character of Linear and non-Linear-ortho-fused polynuclear hydrocarbons, ortho-and peri-fused polynuclear hydrocarbons. General method of preparation and reactions of indene, fluorene anthracene and phenanthrene. Modern methods of synthesis of macro ring compounds-civeton, muscone and catenanes.

**UNIT-II**

**Heterocyclic Synthesis**

Principles of heterocyclic synthesis involving cyclization reactions and cycloaddition reaction.

**Small Ring Heterocycles**

Synthesis of aziridines, oxiranes, thiiranes and their ring opening and rearrangement reactions.

**Five-Membered Heterocycles with one Heteroatom**

Synthesis of Furan, Pyrrole, Thiophene and their electrophilic, nucleophilic, metallation reactions.

**Six-Membered Heterocycles with one Heteroatom**

Pyridine synthesis (from dicarbonyl compounds, Hantzsch Synthesis, *through* cycloaddition reactions), reactions of pyridine (electrophilic, nucleophilic, metallation), synthesis of pyrylium salts, pyrones, benzopyrylium salts, benzopyrones (coumarins, chromones) and their electrophilic, nucleophilic and addition reactions, reactivity of pyrylium and benzopyrylium salts, pyrones and benzopyrones.

**Seven-and Large-Membered Heterocycles**

Synthesis and reactions of azepines, oxepines, thiepinines, thiazepines.

### UNIT-III

#### Reagents in Organic Synthesis

Use of the following reagents in organic synthesis and functional group transformations; Complex metal hydrides, Gilman's reagent, lithium dimethylcuprate, lithium diisopropylamide (LDA) dicyclohexylcarbodiimide. 1,3-Dithiane (reactivity umpolung), trimethylsilyl iodide, tri-n-butyltin hydride, Woodward and Prevost hydroxylation, osmium tetroxide, DDQ, selenium dioxide, phase transfer catalysts, crown ethers and Merrifield resin, Peterson's synthesis, Wilkinson's catalyst, Baker yeast.

### UNIT-IV

#### Supramolecular Chemistry

Definition and development of supramolecular chemistry, Classification of supramolecular Host- Guest compounds, Historical concepts such as receptors, coordination, lock and key analogy, Chelate and Macrocyclic effects, Preorganization and Complementarity, Thermodynamics and Kinetic selectivity, Overview of intermolecular forces such as Hydrogen bonding, Hydrophobic effects, Cation- $\pi$  interactions, Ion-ion, Ion-dipole, Dipole-dipole interactions,  $\pi$ - $\pi$  stacking, van der Waals forces, Synthesis and structure of supramolecular hosts for Recognition of cations: Crown ethers, Cryptands, Spherands, Siderophores; for Recognition of anions: Guanidinium- based receptors; for Recognition of neutral molecules: Cyclotrimeratrylene (CTV).

#### Book Recommended:

1. Supramolecular Chemistry, Jonathan W. Steed, Jerry L. Atwood, John Wiley & Sons
2. Principles of Modern Heterocyclic Chemistry by L.A. Paquette
3. Heterocyclic Chemistry by J.A. Joule and K. Mills
4. Heterocyclic Chemistry by Gilchrist

**Master of Science (Chemistry)**  
**(Semester-III)**  
**Session: 2020-21**  
**COURSE CODE: MCHL-3083**  
**COURSE TITLE: Surface and Polymer Chemistry**  
**(Theory)**

**Course outcomes:**

Students will be able to

CO1: study concept of adsorption and micelle formation

CO2: learn about the different kinetics and thermodynamics of polymerization

CO3: learn about the type and classification of polymers

CO4: know about the structure, properties and utilization of polymers.

CO5: study in detail about the glass transition temperature

**Master of Science (Chemistry)**  
**(Semester-III)**  
**Session: 2020-21**  
**COURSE CODE: MCHL-3083**  
**COURSE TITLE: Surface and Polymer Chemistry (Theory)**

**Time: 3 Hrs**

**Max. Marks: 50**

**(Theory: 40, CA: 10)**

**Note: The students are allowed to use Non-Programmable Calculator.**

**Instructions for the Paper Setters:**

Eight questions of equal marks (eight each) are to be set, two in each of the four Sections (A-D). Questions of Sections A-D should be set from UNITS I-IV of the syllabus respectively. Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each section. The fifth question may be attempted from any Section.

**UNIT-I**

**Adsorption**

Surface tension, capillary action, pressure difference across curved surface (Laplace equations), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, estimation of surface area (BET equation), surface films on liquids (Electro-kinetic phenomena), and catalytic activity at surfaces.

**UNIT-II**

**Micelles**

Surface active agents, classification of surface active agents, micellization, hydrophobic interactions, critical micellar concentration (CMC), factors affecting CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization – phase separation and mass action models, solubilization, micro emulsion, reverse micelles.

**UNIT-III**

**Macromolecules**

**Polymer** – definition, types of polymers, electrically conducting, fire resistant, liquid crystal polymers, kinetics of polymerization, thermodynamics of polymerization.

Molecular mass, number and mass average molecular mass, molecular mass determination (osmometry, viscometry, diffusion and light scattering methods), sedimentation, chain configuration of macromolecules, calculations of average dimensions of various chain structures. Importance of polymers, Basic concepts: monomers, repeat units, degree of polymerization. Linear, branched and network polymers. Classification of polymers. Polymerization: condensation, addition, radical chain-ionic and coordination and copolymerization. Polymerization conditions and polymer reactions. Polymerization in homogeneous and heterogeneous systems. Number, weight and viscosity average weights.

## UNIT IV

### Structure and Properties:

Polymer structure and properties-crystalline melting point  $T_m$ -melting point of homogenous series, effect of chain flexibility and steric factors, entropy and heat of fusion. The glass transition temperature,  $T_g$ -Relationship between  $T_m$  and  $T_g$ , effects of molecular weight, diluents, chemical structure, chain topology, branching and chain linking. Property requirements and polymer utilization.

### Books Recommended:

1. Physical Chemistry, P. W. Atkins.
2. Textbook of polymer science, F. W. Billmeyer Jr. Wiley.
3. Polymer science, V. R. Gowariker, N. V. Viswanathan and J. Sreedhar, Wiley-Eastern
4. Polymer Chemistry, Melcolm P. Stevens, Oxford University Press
5. Physical Chemistry of Polymers , A.Tager, Mir Publishers, Moscow



**Master of Science (Chemistry)**  
**(Semester-III)**  
**Session: 2020-21**  
**COURSE CODE: MCHL-3084**  
**COURSE TITLE: Electrochemistry and Chemical Dynamics (Theory)**

**Course outcomes:**

Students will be able to

CO1: Understand the electrochemistry of solutions, method of determination of electrified interfaces, semiconductor electrolyte solution interface

CO2: know theory, monitoring and prevention of corrosion

CO4: understand collision theory of reaction rates, Arrhenius theory and activated complex theory, Lindemann-Hinshelwood theory

CO5: understand various Photochemical reactions, Homogeneous catalysis and kinetics of enzyme reactions, general features and methods of studying fast reactions

CO6: interpret spectra and applications of Voltammetry and Polarography.

**Master of Science (Chemistry)**  
**(Semester-III)**  
**Session: 2020-21**  
**COURSE CODE: MCHL-3084**  
**COURSE TITLE: Electrochemistry and Chemical Dynamics (Theory)**

**Time: 3 Hrs**

**Max. Marks: 50**

**(Theory: 40, CA: 10)**

**Note: The students are allowed to use Non-Programmable Calculator.**

**Instructions for the Paper Setters:**

Eight questions of equal marks (eight each) are to be set, two in each of the four Sections (A-D). Questions of Sections A-D should be set from UNITs I-IV of the syllabus respectively. Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each section. The fifth question may be attempted from any Section.

**UNIT-I**

**Electrochemistry** Electrochemistry of solutions, Debye-Huckel-Onsager treatment and its extension, ion-solvent interactions, Debye-Huckel-Bjerrum mode, Thermodynamics of electrified interface equation, Derivation of electro-capillarity, Lipmann equation(surface excess), method of determination, structure of electrified interfaces, Guoy-Chapman, Stern models, over potential, exchange current density, derivation of Butler-Volmer equation, Tafel plot.

Semiconductor interface theory of double layer at semiconductor electrolyte solution interface, structure of double layer interfaces, effect of light at semiconductor solution interface.

Introduction to corrosion, homogeneous theory, forms of corrosion, corrosion monitoring and prevention

**UNIT-II**

**Chemical Dynamics (A)**

Methods of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius theory and activated complex theory, ionic reactions, kinetic salt effects,, treatment of unimolecular reactions, Lindemann-Hinshelwood theory. Dynamic Chain (hydrogen bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane),

**UNIT-III**

**Chemical Dynamics (B)**

Photochemical reactions between hydrogen-bromine and hydrogen-chlorine, oscillatory reactions (Belousov-Zhabotinsky reactions), Homogeneous catalysis and kinetics of enzyme reactions, general features of fast reactions, study of fast reactions by flow method, relaxation method, flash photolysis, nuclear resonance.

**UNIT-IV**

**Voltammetry and Polarography**

Polarography, polarographic cells, polarogram, interpretation of polarographic waves, equation for the polarographic waves, effect of complex formation on polarographic wave, polarograms for irreversible reactions, dropping mercury electrode, current variations during life time of a drop, merits and demerits

of dme, polarographic diffusion currents, Ilkovic equation, capillary characteristics, temperature, polarograms for mixture of reactants, anodic and cathodic waves, factors affecting polarographic currents, applications of polarography, treatment of data, organic and inorganic polarographic analysis, voltammetry at solid electrodes, cyclic voltammetry and interpretation of data, , pilot-ion and standard addition method for quantitative analysis

**Books Recommended:**

1. Chemical Kinetics, K. J. Laddler, McGraw-Hill
2. Modern Electrochemistry Vol.1,2,3, J. Bochriss and A.K.N. Reddy
3. Fundamentals of electrochemistry; P. Monk
4. Principles of Instrumental Analysis; Skoog, West; Saunders Publications

**Master of Science (Chemistry)**  
**(Semester-III)**  
**Session: 2020-21**  
**COURSE CODE: MCHL-3085**  
**COURSE TITLE: Photochemistry and Pericyclic reactions (Theory)**

**Course outcomes:**

Students will be able to

CO1: classify the pericyclic reactions and explain them under thermal and photochemical conditions.

CO2: interpret the product of Pericyclic reactions (Cyclo addition, Electrocyclic and sigmatropic Reactions)

CO3: know the basic concepts of photochemical reactions and determine their reaction mechanisms

CO4: apply the knowledge of photochemical reactions of Alkenes, carbonyl compounds, aromatic compounds.

CO5: study named photochemical reactions, photochemistry of smog, polymers and vision

**Master of Science (Chemistry)**  
**(Semester-III)**  
**Session: 2020-21**  
**COURSE CODE: MCHL-3085**  
**COURSE TITLE: Photochemistry and Pericyclic reactions (Theory)**

**Time: 3 Hrs**

**Max. Marks: 50**

**(Theory: 40, CA: 10)**

**Note: The students are allowed to use Non-Programmable Calculator.**

**Instructions for the Paper Setters:**

Eight questions of equal marks (eight each) are to be set, two in each of the four Sections (A-D). Questions of Sections A-D should be set from UNITs I-IV of the syllabus respectively. Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each section. The fifth question may be attempted from any Section.

**UNIT-1**

**Pericyclic Reactions (A)**

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene, allyl system, classification of pericyclic reactions FMO approach. Woodward-Hoffmann correlation diagrams method and Perturbation of molecular orbital (PMC) approach for the explanation of pericyclic reactions under thermal and photo-chemical conditions. Electrocyclic reactions – conrotatory and disrotatory motions,  $4n$ ,  $4n+2$ , allyl systems secondary effects. Cycloadditions – antarafacial and suprafacial additions, notation of cycloadditions ( $4n$ ) and ( $4n+2$ ) systems with a greater emphasis on ( $2+2$ ) and ( $4+2$ )

**UNIT-II**

**Pericyclic Reactions (B)**

cycloaddition-stereochemical effects and effects of substituents on the rates of cycloadditions, 1,3-dipolar cyclo-additions and cheletropic reactions. Sigmatropic Rearrangements-suprafacial and antarafacial shifts [1,2]- sigmatropic shifts involving carbon moieties retention and inversion of configuration, (3,3) and (5,5) sigma-tropic rearrangements, detailed treatment of Claisen and Cope rearrangements, fluxional tautomerism, aza-cope rearrangements, introductions to Ene reactions, simple problems on pericyclic reactions. Electrocyclic rearrangement of cyclobutenes and 1,3 cyclohexadienes.

**UNIT-III**

**Photochemistry**

Interaction of electromagnetic radiation with matter, types of excitations, fate of excited molecule, quantum yield, transfer of excitation energy, actinometry.

**Determination of Reaction Mechanism**

Classification, rate constants and life times of reactive energy states –determination of rate constants of reactions. Effect of light intensity on the rate of photochemical reactions. Types of photochemical reactions – photodissociation, gas-phase photolysis.

#### **UNIT-IV**

##### **Photochemistry of Alkenes**

Intramolecular reactions of the olefinic bond – geometrical isomerism, cyclisation reactions, rearrangement of 1,4- and 1,5-dienes.

##### **Photochemistry of Carbonyl Compounds**

Intramolecular reactions of carbonyl compounds – saturated, cyclic and acyclic,  $\beta$ ,  $\gamma$ -unsaturated and  $\alpha,\beta$ -unsaturated compounds, Cyclohexadienones. Intermolecular cycloaddition reactions – dimerisations and oxetane formation.

##### **Photochemistry of Aromatic Compounds**

Isomerisations, additions and substitutions.

##### **Miscellaneous Photochemical Reactions**

Photo-Fries reactions of anilides. Photo-Fries rearrangement. Barton reaction. Singlet molecular oxygen reactions. Photochemical formation of smog. Photodegradation of polymers. Photochemistry of vision.

#### **Books Recommended:**

1. Organic Photochemistry – Chapman and Depuy.
2. Organic Photochemistry – W.H. Horsepool.
3. Photochemistry of Excited States – J.D.Goyle.
4. Pericyclic Reactions: A Mechanistic study by S.M. Mukherji
5. The conservation of orbital Symmetry by R. B. Woodward and R. Hoffman
6. Fundamentals of Photochemistry by K.K.Rohtagi Mukherji

**Master of Science (Chemistry)**  
**(Semester-III)**  
**Session: 2020-21**  
**COURSE CODE: MCHP-3086**  
**COURSE TITLE: Inorganic Chemistry Practical (Preparations)**

**Course outcomes:**

Students will be able to

CO1: plan and Conduct experiments for synthesizing, analysing, identifying and characterizing inorganic compounds

CO2: do measurements of magnetic moments of synthesized complexes.

CO3: estimate metal content in the synthesized complex

**Master of Science (Chemistry)**  
**(Semester-III)**  
**Session: 2020-21**  
**COURSE CODE: MCHP-3086**  
**COURSE TITLE: Inorganic Chemistry Practical (Preparations)**

**Time: 6 hrs.**

**Max. Marks: 75**  
**(P: 60, CA: 15)**

**Instruction for practical examiner:** Question paper is to be set on the spot jointly by the Internal and External Examiners. Two copies of the same should be submitted for the record to COE Office, Kanya Maha Vidyalaya, Jalandhar.

1. Preparation of  $\text{Co}(\text{acac})_3$ , its characterization using NMR, IR, UV-Vis and analysis of Cobalt. (ref. J. Chem. Edu., 1980, 57, 7, 525)
2. Preparation of  $\text{Co}(\text{acac-NO}_2)_3$ , its characterization using NMR, IR, UV-Vis and analysis of Cobalt. (ref. J. Chem. Edu., 1980, 57, 7, 525)
3. Preparation of  $[\text{Fe}(\text{H}_2\text{O})_6][\text{Fe}(\text{N-salicylideneglycinato})_2]_2 \cdot 3\text{H}_2\text{O}$ , its characterization using IR, UV-Vis, magnetic susceptibility and analysis of Iron. (ref. Inorganica Chimica Acta, 1977, 23, 35).
4. Preparation of  $[\text{Ni}(\text{NH}_3)_6]\text{Cl}_2$  its characterization using IR, UV-Vis, magnetic susceptibility and analysis of Nickel and  $\text{NH}_3$ . (ref. Marr and Rockett, 1972).
5. Preparation of  $[\text{Ni}(\text{ethylenediamine})_3]\text{Cl}_2$  its characterization using IR, UV-Vis, magnetic susceptibility and analysis of Nickel. (ref. Marr and Rockett, 1972, page 270).
6. Preparation of  $[\text{Fe}(\text{NO})(\text{S}_2\text{CN}(\text{Et})_2)_2]$  its characterization using IR, UV-Vis, magnetic susceptibility and analysis of Fe(II). (ref. Marr and Rockett, 1972, page 262, J. Chem. Soc. 1962, 84, 3404).
7. Preparation of octahedral and tetrahedral complexes of dichlorodipyridylcobalt(II), differentiate them using IR, UV and magnetic properties. Estimate Co(II) from one of them. (ref. Marr and Rockett, 1972, page 375, Inorganic Chemistry, 1966, 5, 615).
8. Preparation of  $\text{VO}(\text{acac})_2$  and its piperidine complex, characterize using IR, UV and magnetic moment. Estimate for V(IV). (ref. Marr and Rockett, 1972, 243).
9. Preparation of diaquotetraacetataocopper(II), magnetic susceptibility IR and UV-Vis, analysis of Copper(II).
10. Preparation of cis- and trans- potassium dioxalato diaquochromate(III). Interpretation of IR, UV and magnetic properties. Estimation of Chromium. (ref. Marr and Rockett, 1972, page 386).
11. Preparation of  $\text{HgCo}(\text{NCS})_4$ , its IR and measure its magnetic moment. (ref. Marr and Rockett, 1972, page 365).



12. Preparation of sodium tetrathionate, interpretation of its IR and analysis using potassium iodate. (ref. Marr and Rockett, 1972, page 214).
13. Preparation of Potassium dithionate, interpretation of its IR and analysis using potassium iodate. (ref. Marr and Rockett, 1972, page 214).
14. Preparation of bis(acetylacetonato)copper(II), UV-Vis, and IR, magnetic studies, Demonstration of Jahn Teller effect by solution spectral studies. (ref. Bull. Chem. Soc. Japan, 1965, 29, 852).
15. Preparation of salicylamide complexes of Copper(II). IR, UV, magnetic data and analysis of Cu(II). (ref. Indian J. of Chem., 1977, 15A, No. 5, 459; *ibid*, 1971, 9, 1396).
16. To prepare a macrocyclic ligand 5,7,7,12,14,14-hexamethyl-1,4,8,11-tetraazacyclo tetradeca-4,11-dienedi(hydrogeniodide) and its complex with Ni(II). Study IR, NMR and UV-Vis of ligand and complex and magnetic properties of complex. To analyze for Ni and I. (J. Chem. Edu. 1977, 79, 581).
17. Preparation and resolution of tris (ethylenediamine) cobalt (III). UV-Vis, NMR, IR, optical rotation of the resolved complexes. ((ref. Marr and Rockett, 1972, page 386).

### **Books Recommended:**

1. B.N. Figgis, Introduction to Ligand Field, Wiley Eastern.
2. A.B.P. Lever, Inorganic Electronic Spectroscopy, Elsevier.
3. A.Earnshaw, Introduction to Magnetochemistry, Academic Press.
4. J.E. Huheey, Inorganic Chemistry Principles of Structure and Reactivity, Harper Interscience.
5. R.S. Drago, Physical Method in Chemistry, W.B.Saunders Company.
6. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, Wiley Interscience.
7. F.A. Cotton, Chemical Application of Group Theory, Wiley Easter

**Master of Science (Chemistry)**  
**(Semester-III)**  
**Session: 2020-21**  
**COURSE CODE: MCHP-3087**  
**COURSE TITLE: Physical Chemistry Practical**

**Course outcomes**

Students will be able to

CO1: apply the principle and mechanism of Conductometric and potentiometric titrations

CO2: determine the partial molar volume of compounds using Dilatometer

CO3: determine specific and molar refractivity using Abbes refractometer

CO4: study complex formation and the kinetics of hydrolysis Spectrophotometrically

CO5: determine the molecular weight of polymers by viscometry

**Master of Science (Chemistry)**  
**(Semester-III)**  
**Session: 2020-21**  
**COURSE CODE: MCHP-3087**  
**COURSE TITLE: Physical Chemistry Practical**

**Time: 6 hrs.**

**Max. Marks: 75**  
**(P: 60, CA: 15)**

**Instruction for practical examiner:** Question paper is to be set on the spot jointly by the Internal and External Examiners. Two copies of the same should be submitted for the record to COE Office, Kanya Maha Vidyalaya, Jalandhar.

1. To determine the partial molar volume of  
(a) Glycine (b) Urea using dilatometer
2. To determine the partial molar volume of  
(a) methanol (b) n-propanol using dilatometer
3. To determine the surface tension (double capillary) of mixture of solid and water by differential method and hence find out parachor of the mixture.
4. To determine the specific and molar refractivity of n-propanol, butanol, hexane and carbon tetrachloride and calculate refraction equivalents of C, H and Cl.
5. To determine the molar refractivity of water, DMF, Dioxane and mixtures of water-DMF, water-Dioxane and verify the refractivity rule. Predict about the interactions between components of mixture by plotting graph between refractive index and mole fraction.
6. To determine the equivalent conductance of weak electrolyte (acetic acid) at infinite dilution using Kohlrausch law.
7. Determine equivalent conductance of strong electrolyte at several concentrations and hence verify Onsager equation.
8. Determine equivalent conductance of weak electrolyte, say acetic acid at different concentrations and hence test validity of Ostwald's dilution law. Also determine dissociation constant of the electrolyte.
9. To determine dissociation constant of a dibasic acid potentiometrically.
10. To study complex formation between Fe (III) and salicylic acid and find out the formula of the complex spectrophotometrically.
11. To determine the formula of the complex ion formed between Fe (III) and thiocyanate ion by Job's method.
12. To study the kinetics of hydrolysis of crystal violet spectrophotometrically.
13. To determine the pH of various mixtures of sodium acetate and acetic acid in aqueous solution and hence determine the dissociation constant of the acid.
14. Titrate potentiometrically Zn(II) by  $K_4Fe(CN)_6$  and verify the composition of the complex  $K_2Zn_3[Fe(CN)_6]_2$
15. Determination of nitrite in water spectrophotometrically.
16. Determination of molecular weight of polymers by Viscometry.

17. Determine the molar refraction of a solid substance by dissolving it in a solvent and its refractive index.

**Books Recommended:**

1. Yadav, J. B (2005): *Advanced Practical Physical Chemistry*, 22<sup>nd</sup> edition, Goel publishing House, Krishna Prakashan Media Ltd.
2. Venkatesan, V., Veeraswamy, R. and Kulandaivelu, A.R (1997): *Basic Principles of Practical Chemistry*”, 2nd edition, Sultan Chand and Sons Publication, New Delhi.